SYSTEM, METHOD AND COMPUTER PROGRAM PRODUCT FOR IDENTIFYING CHEMICAL COMPOUNDS HAVING DESIRED PROPERTIES

ABSTRACT

A system, method, and computer program product for visualizing and interactively analyzing data relating to chemical compounds. A user selects a plurality of compounds to map, and also selects a method for evaluating similarity/dissimilarity between the selected compounds. A non-linear map is generated in accordance with the selected compounds and the selected method. The non-linear map has a point for each of the selected compounds, wherein a distance between any two points is representative of similarity/dissimilarity between the corresponding compounds. A portion of the non-linear map is then displayed. Users are enabled to interactively analyze compounds represented in the non-linear map.

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